



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:07 AM UTC

PDB ID : 4NC3 / pdb_00004nc3
Title : Crystal structure of the 5-HT_{2B} receptor solved using serial femtosecond crystallography in lipidic cubic phase.
Authors : Liu, W.; Wacker, D.; Gati, C.; Han, G.W.; James, D.; Wang, D.; Nelson, G.; Weierstall, U.; Katritch, V.; Barty, A.; Zatsepin, N.A.; Li, D.; Messerschmidt, M.; Boutet, S.; Williams, G.J.; Koglin, J.E.; Seibert, M.M.; Wang, C.; Shah, S.T.A.; Basu, S.; Fromme, R.; Kupitz, C.; Rendek, K.N.; Grotjohann, I.; Fromme, P.; Kirian, R.A.; Beyerlein, K.R.; White, T.A.; Chapman, H.N.; Caffrey, M.; Spence, J.C.H.; Stevens, R.C.; Cherezov, V.; GPCR Network (GPCR)
Deposited on : 2013-10-23
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)

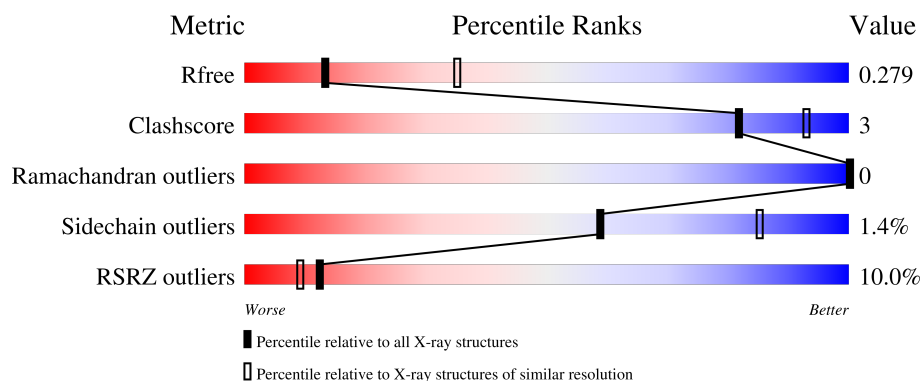
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	430	9% 80% 6% 14%

CCP4 : 9.0.010 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 3123 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

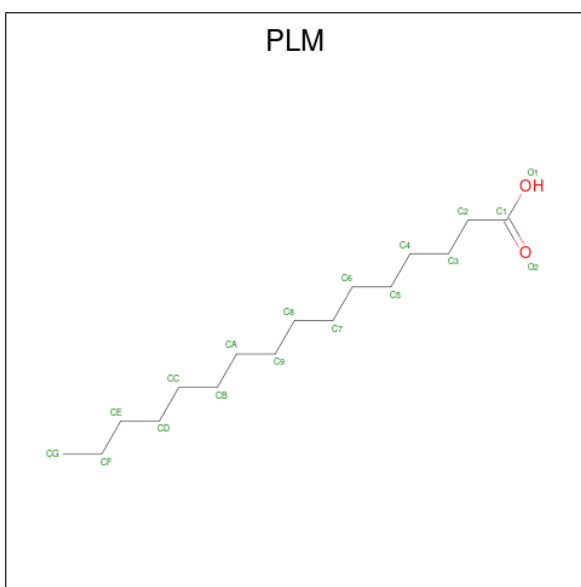
- Molecule 1 is a protein called Chimera protein of human 5-hydroxytryptamine receptor 2B and E. Coli soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	1	0
			2839	1867	451	505	16			

There are 23 discrepancies between the modelled and reference sequences:

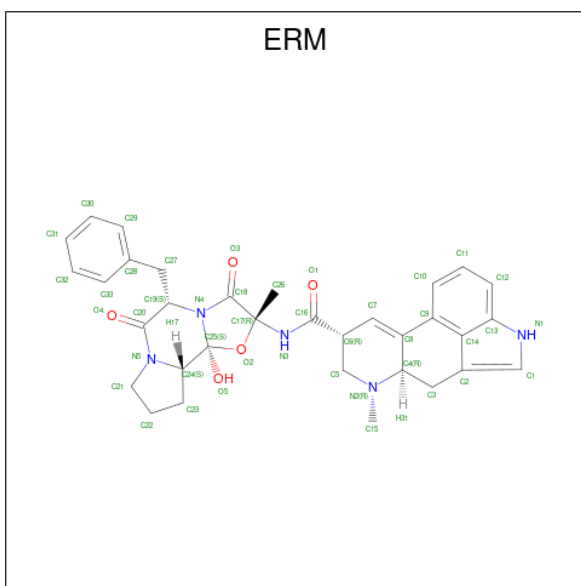
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ASP	-	expression tag	UNP P41595
A	27	TYR	-	expression tag	UNP P41595
A	28	LYS	-	expression tag	UNP P41595
A	29	ASP	-	expression tag	UNP P41595
A	30	ASP	-	expression tag	UNP P41595
A	31	ASP	-	expression tag	UNP P41595
A	32	ASP	-	expression tag	UNP P41595
A	33	GLY	-	expression tag	UNP P41595
A	34	ALA	-	expression tag	UNP P41595
A	35	PRO	-	expression tag	UNP P41595
A	144	TRP	MET	engineered mutation	UNP P41595
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	406	GLY	-	expression tag	UNP P41595
A	407	ARG	-	expression tag	UNP P41595
A	408	PRO	-	expression tag	UNP P41595
A	409	LEU	-	expression tag	UNP P41595
A	410	GLU	-	expression tag	UNP P41595
A	411	VAL	-	expression tag	UNP P41595
A	412	LEU	-	expression tag	UNP P41595
A	413	PHE	-	expression tag	UNP P41595
A	414	GLN	-	expression tag	UNP P41595

- Molecule 2 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	16	1		

- Molecule 3 is Ergotamine (CCD ID: ERM) (formula: $C_{33}H_{35}N_5O_5$).



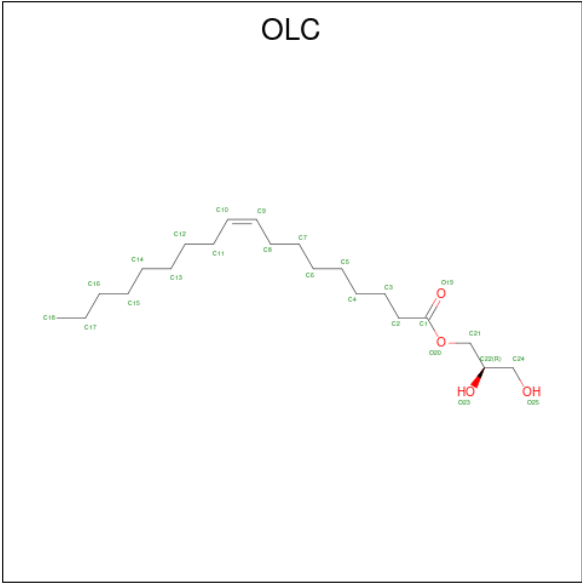
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			43	33	5	5		

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



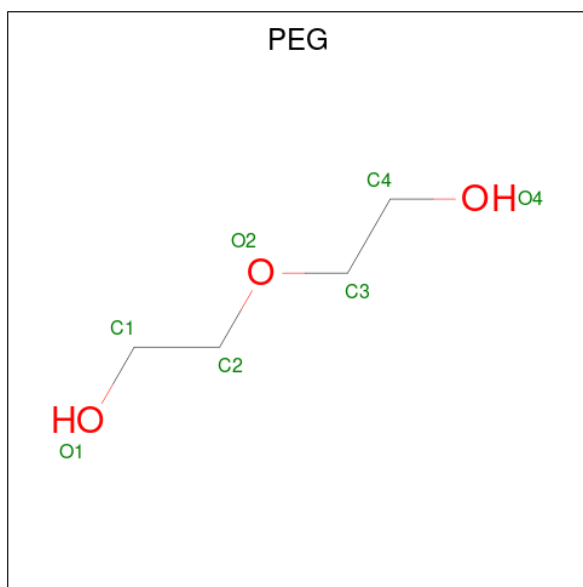
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	15	4		
5	A	1	Total	C	O	0	0
			16	12	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			19	15	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



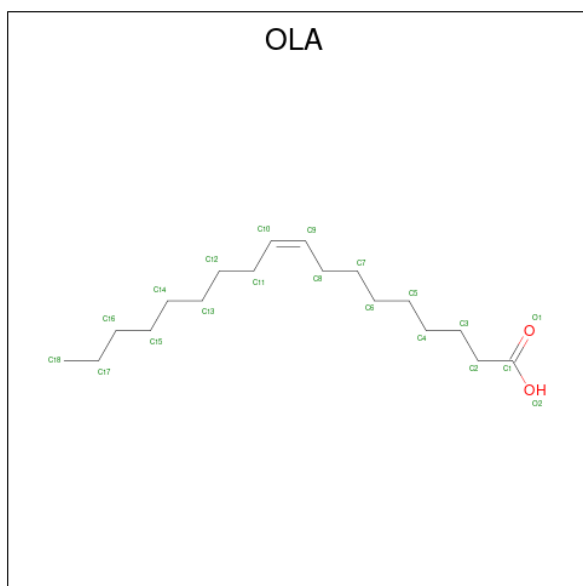
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



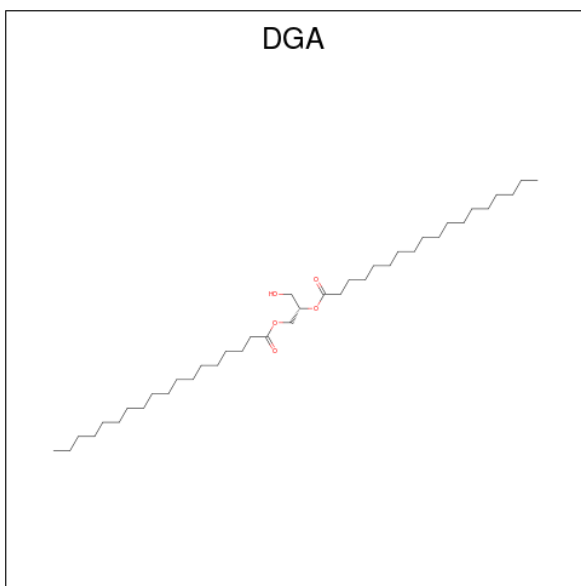
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C		0	0
			10	10			
8	A	1	Total	C	O	0	0
			20	18	2		
8	A	1	Total	C	O	0	0
			19	17	2		

- Molecule 9 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			26	21	5		
9	A	1	Total	C	O	0	0
			20	15	5		

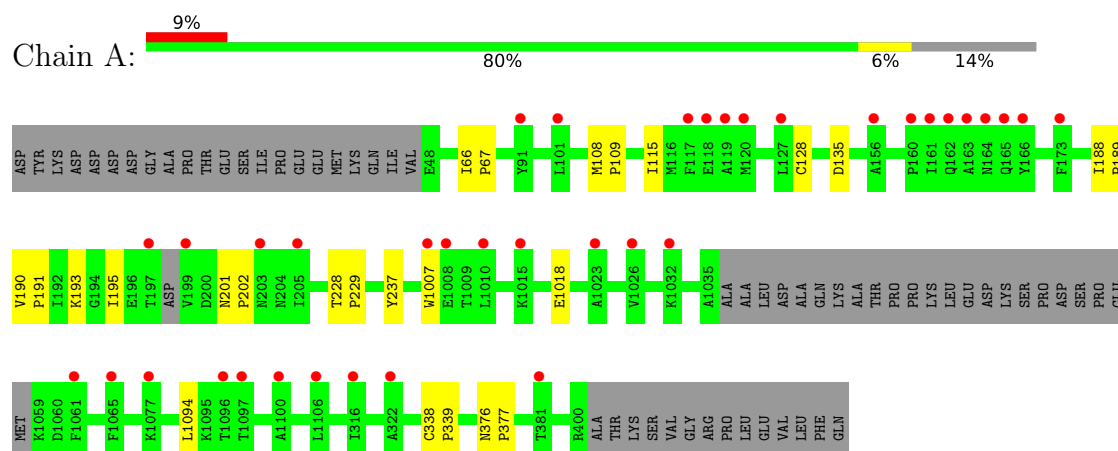
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	7	Total	O	0	0
			7	7		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Chimera protein of human 5-hydroxytryptamine receptor 2B and E. Coli soluble cytochrome b562



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	61.50Å 122.20Å 168.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.68 – 2.80 34.68 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.68-2.80) 99.9 (34.68-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.94 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.227 , 0.270 0.245 , 0.279	Depositor DCC
R_{free} test set	1078 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	106.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 138.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3123	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, OLA, ERM, OLC, DGA, TRS, PLM, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/2903	0.66	0/3965

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2839	0	2823	13	0
2	A	17	0	31	0	0
3	A	43	0	35	0	0
4	A	28	0	46	1	0
5	A	79	0	111	3	0
6	A	7	0	9	0	0
7	A	8	0	12	0	0
8	A	49	0	76	0	0
9	A	46	0	56	0	0
10	A	7	0	0	0	0
All	All	3123	0	3199	16	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:CYS:SG	1:A:195:ILE:CD1	2.84	0.65
1:A:201:ASN:HB3	1:A:202:PRO:HD3	1.84	0.58
1:A:188:ILE:N	1:A:189:PRO:CD	2.70	0.55
1:A:1007:TRP:C	1:A:1007:TRP:CD1	2.86	0.53
1:A:376:ASN:HB3	1:A:377:PRO:HD3	1.92	0.52
1:A:135:ASP:C	1:A:135:ASP:OD1	2.53	0.51
4:A:1203:CLR:H183	4:A:1203:CLR:H212	1.91	0.51
5:A:1207:OLC:C14	5:A:1207:OLC:H18A	2.42	0.49
1:A:237:TYR:HA	5:A:1204:OLC:H22	1.97	0.46
1:A:201:ASN:HB3	1:A:202:PRO:CD	2.47	0.44
1:A:66:ILE:HB	1:A:67:PRO:HD3	2.00	0.44
5:A:1207:OLC:H18A	5:A:1207:OLC:H14	1.99	0.43
1:A:338:CYS:N	1:A:339:PRO:CD	2.82	0.42
1:A:228:THR:HB	1:A:229:PRO:CD	2.50	0.42
1:A:108:MET:HB2	1:A:109:PRO:HD3	2.02	0.42
1:A:190:VAL:HB	1:A:191:PRO:CD	2.50	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/430 (85%)	352 (96%)	13 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	293/371 (79%)	289 (99%)	4 (1%)	59 85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ILE
1	A	193	LYS
1	A	1018	GLU
1	A	1094	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OLC	A	1207	-	24,24,24	1.06	2 (8%)	25,25,25	1.12	2 (8%)
6	PEG	A	1206	-	6,6,6	0.60	0	5,5,5	0.24	0
5	OLC	A	1204	-	18,18,24	1.21	2 (11%)	19,19,25	1.03	1 (5%)
8	OLA	A	1210	-	9,9,19	0.98	1 (11%)	8,8,19	0.65	0
8	OLA	A	1212	-	18,18,19	0.83	1 (5%)	18,18,19	0.94	1 (5%)
9	DGA	A	1214	-	19,19,43	1.09	2 (10%)	21,21,45	1.43	3 (14%)
5	OLC	A	1205	-	15,15,24	1.25	2 (13%)	16,16,25	1.11	1 (6%)
3	ERM	A	1202	-	50,50,50	1.23	8 (16%)	73,79,79	1.96	19 (26%)
2	PLM	A	1201	1	16,16,17	0.85	1 (6%)	15,15,17	0.57	0
5	OLC	A	1208	-	18,18,24	1.20	2 (11%)	19,19,25	1.12	2 (10%)
8	OLA	A	1211	-	19,19,19	0.81	1 (5%)	19,19,19	0.88	0
4	CLR	A	1203	-	31,31,31	0.68	1 (3%)	48,48,48	1.73	13 (27%)
7	TRS	A	1209	-	7,7,7	0.31	0	9,9,9	0.48	0
9	DGA	A	1213	-	25,25,43	0.97	2 (8%)	27,27,45	1.29	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLC	A	1207	-	-	13/24/24/24	-
6	PEG	A	1206	-	-	1/4/4/4	-
5	OLC	A	1204	-	-	9/18/18/24	-
8	OLA	A	1210	-	-	4/7/7/17	-
8	OLA	A	1212	-	-	11/16/16/17	-
9	DGA	A	1214	-	-	13/21/21/45	-
5	OLC	A	1205	-	-	5/15/15/24	-
3	ERM	A	1202	-	-	0/13/87/87	0/8/8/8
2	PLM	A	1201	1	-	6/14/14/15	-
5	OLC	A	1208	-	-	8/18/18/24	-
8	OLA	A	1211	-	-	13/17/17/17	-
4	CLR	A	1203	-	-	5/10/68/68	0/4/4/4
7	TRS	A	1209	-	-	2/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	DGA	A	1213	-	-	14/27/27/45	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1205	OLC	O20-C1	3.55	1.43	1.33
5	A	1204	OLC	O20-C1	3.52	1.43	1.33
5	A	1207	OLC	O20-C1	3.51	1.43	1.33
5	A	1208	OLC	O20-C1	3.50	1.43	1.33
2	A	1201	PLM	O1-C1	-3.26	1.25	1.42
3	A	1202	ERM	C12-C13	-2.87	1.35	1.39
8	A	1210	OLA	C10-C9	2.87	1.47	1.29
8	A	1211	OLA	C10-C9	2.78	1.47	1.31
8	A	1212	OLA	C10-C9	2.77	1.47	1.31
9	A	1214	DGA	OG1-CA1	2.60	1.40	1.33
9	A	1214	DGA	OG2-CB1	2.60	1.41	1.34
9	A	1213	DGA	OG1-CA1	2.59	1.40	1.33
9	A	1213	DGA	OG2-CB1	2.59	1.41	1.34
5	A	1204	OLC	C2-C1	2.57	1.58	1.50
5	A	1208	OLC	C2-C1	2.57	1.58	1.50
3	A	1202	ERM	C19-N4	-2.52	1.43	1.47
5	A	1207	OLC	C2-C1	2.47	1.57	1.50
5	A	1205	OLC	C2-C1	2.43	1.57	1.50
3	A	1202	ERM	C3-C4	2.30	1.57	1.53
3	A	1202	ERM	C6-C16	2.29	1.56	1.53
3	A	1202	ERM	C11-C12	2.27	1.42	1.38
3	A	1202	ERM	C27-C19	-2.19	1.50	1.54
3	A	1202	ERM	C5-N2	2.15	1.50	1.47
4	A	1203	CLR	C10-C9	-2.13	1.52	1.56
3	A	1202	ERM	C24-N5	-2.11	1.44	1.47

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	ERM	O2-C25-N4	-5.70	98.94	104.00
3	A	1202	ERM	C25-O2-C17	5.13	114.49	111.29
3	A	1202	ERM	C25-N4-C18	5.06	117.70	112.64
3	A	1202	ERM	C6-C16-N3	5.02	120.54	114.58
3	A	1202	ERM	C23-C24-N5	4.77	107.90	102.73
4	A	1203	CLR	C3-C4-C5	-3.85	105.92	112.05
9	A	1214	DGA	OG2-CB1-CB2	3.76	119.61	111.48
9	A	1213	DGA	OG2-CB1-CB2	3.72	119.54	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1203	CLR	C1-C2-C3	3.71	115.40	110.48
3	A	1202	ERM	C21-N5-C24	-3.68	105.87	111.57
4	A	1203	CLR	C16-C17-C20	-3.67	106.62	112.18
4	A	1203	CLR	C19-C10-C9	-3.35	107.91	111.66
4	A	1203	CLR	C21-C20-C22	-3.20	105.38	110.34
3	A	1202	ERM	C19-N4-C18	-3.19	122.50	125.93
3	A	1202	ERM	C23-C24-C25	-3.09	114.44	117.65
3	A	1202	ERM	O5-C25-N4	-3.05	110.23	112.86
3	A	1202	ERM	O2-C25-C24	3.00	114.08	110.37
5	A	1205	OLC	O20-C1-C2	2.87	120.60	111.83
4	A	1203	CLR	C18-C13-C14	-2.81	106.58	111.68
5	A	1208	OLC	O20-C1-C2	2.78	120.31	111.83
3	A	1202	ERM	C10-C9-C14	-2.74	116.30	120.16
9	A	1214	DGA	OG1-CA1-CA2	2.73	120.14	111.83
4	A	1203	CLR	C1-C10-C5	2.70	113.40	108.74
5	A	1207	OLC	O20-C1-C2	2.64	119.88	111.83
5	A	1204	OLC	O20-C1-C2	2.63	119.84	111.83
3	A	1202	ERM	C24-C25-N4	2.62	110.96	108.13
9	A	1213	DGA	OG1-CA1-CA2	2.54	119.58	111.83
3	A	1202	ERM	O4-C20-N5	-2.54	119.37	123.00
4	A	1203	CLR	C7-C8-C14	-2.46	107.44	110.93
3	A	1202	ERM	O1-C16-C6	-2.40	118.85	121.44
4	A	1203	CLR	C15-C14-C8	-2.30	115.44	119.10
5	A	1207	OLC	O20-C1-O19	-2.26	117.97	123.63
3	A	1202	ERM	C12-C13-N1	2.23	134.31	130.74
3	A	1202	ERM	C5-N2-C4	2.22	113.49	110.96
4	A	1203	CLR	C13-C14-C8	-2.18	111.32	114.41
4	A	1203	CLR	C11-C9-C10	-2.15	110.44	113.08
4	A	1203	CLR	C13-C17-C20	-2.14	116.18	119.50
3	A	1202	ERM	C25-C24-N5	-2.12	106.52	109.01
3	A	1202	ERM	C14-C13-N1	-2.11	103.65	106.88
4	A	1203	CLR	C2-C1-C10	2.09	117.24	112.78
5	A	1208	OLC	O20-C1-O19	-2.08	118.42	123.63
8	A	1212	OLA	O2-C1-C2	2.05	120.47	114.00
3	A	1202	ERM	C21-N5-C20	2.03	126.61	123.07
9	A	1214	DGA	OG2-CB1-OB1	-2.02	118.98	123.70

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1204	OLC	C21-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
5	A	1205	OLC	C21-C22-C24-O25
5	A	1207	OLC	C21-C22-C24-O25
5	A	1207	OLC	O20-C21-C22-O23
5	A	1208	OLC	O20-C21-C22-C24
5	A	1208	OLC	O20-C21-C22-O23
9	A	1214	DGA	CG1-CG2-CG3-OXT
9	A	1214	DGA	OG2-CG2-CG3-OXT
9	A	1214	DGA	OA1-CA1-OG1-CG1
5	A	1207	OLC	C2-C1-O20-C21
9	A	1214	DGA	CA2-CA1-OG1-CG1
4	A	1203	CLR	C16-C17-C20-C22
5	A	1207	OLC	O19-C1-O20-C21
9	A	1213	DGA	OG1-CG1-CG2-OG2
5	A	1205	OLC	C1-C2-C3-C4
5	A	1205	OLC	O20-C21-C22-O23
5	A	1208	OLC	C3-C4-C5-C6
8	A	1212	OLA	C12-C13-C14-C15
5	A	1204	OLC	O23-C22-C24-O25
5	A	1207	OLC	O23-C22-C24-O25
9	A	1214	DGA	CA3-CA4-CA5-CA6
8	A	1211	OLA	C13-C14-C15-C16
9	A	1214	DGA	CB2-CB1-OG2-CG2
9	A	1213	DGA	CB2-CB3-CB4-CB5
8	A	1211	OLA	C3-C4-C5-C6
8	A	1212	OLA	C6-C7-C8-C9
9	A	1213	DGA	CA2-CA1-OG1-CG1
5	A	1207	OLC	C11-C10-C9-C8
5	A	1204	OLC	C1-C2-C3-C4
8	A	1210	OLA	C4-C5-C6-C7
9	A	1213	DGA	CB7-CB8-CB9-CAB
9	A	1213	DGA	CB2-CB1-OG2-CG2
8	A	1212	OLA	C13-C14-C15-C16
9	A	1213	DGA	CB6-CB7-CB8-CB9
8	A	1212	OLA	C5-C6-C7-C8
5	A	1204	OLC	C11-C10-C9-C8
9	A	1213	DGA	CB4-CB5-CB6-CB7
5	A	1205	OLC	O23-C22-C24-O25
9	A	1213	DGA	CB9-CAB-CBB-CCB
8	A	1211	OLA	C10-C11-C12-C13
8	A	1212	OLA	C3-C4-C5-C6
2	A	1201	PLM	CB-CC-CD-CE
2	A	1201	PLM	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	A	1211	OLA	C11-C10-C9-C8
8	A	1212	OLA	C4-C5-C6-C7
8	A	1211	OLA	C15-C16-C17-C18
2	A	1201	PLM	C8-C9-CA-CB
8	A	1211	OLA	C4-C5-C6-C7
9	A	1213	DGA	CA2-CA3-CA4-CA5
8	A	1211	OLA	C14-C15-C16-C17
9	A	1214	DGA	CA5-CA6-CA7-CA8
5	A	1207	OLC	C5-C6-C7-C8
8	A	1212	OLA	C11-C10-C9-C8
7	A	1209	TRS	N-C-C1-O1
9	A	1213	DGA	OG1-CG1-CG2-CG3
9	A	1214	DGA	OG1-CG1-CG2-CG3
5	A	1207	OLC	C10-C11-C12-C13
5	A	1207	OLC	O20-C21-C22-C24
8	A	1211	OLA	C11-C12-C13-C14
5	A	1207	OLC	C15-C16-C17-C18
5	A	1207	OLC	C1-C2-C3-C4
9	A	1214	DGA	OG1-CG1-CG2-OG2
5	A	1205	OLC	C2-C3-C4-C5
9	A	1213	DGA	OA1-CA1-OG1-CG1
7	A	1209	TRS	C3-C-C1-O1
5	A	1208	OLC	C5-C6-C7-C8
8	A	1212	OLA	C11-C12-C13-C14
4	A	1203	CLR	C16-C17-C20-C21
5	A	1204	OLC	C9-C10-C11-C12
5	A	1208	OLC	C9-C10-C11-C12
2	A	1201	PLM	CC-CD-CE-CF
8	A	1210	OLA	C5-C6-C7-C8
5	A	1208	OLC	C2-C1-O20-C21
4	A	1203	CLR	C13-C17-C20-C22
5	A	1204	OLC	C7-C8-C9-C10
9	A	1213	DGA	OB1-CB1-OG2-CG2
8	A	1210	OLA	C1-C2-C3-C4
8	A	1210	OLA	C7-C8-C9-C10
8	A	1211	OLA	C12-C13-C14-C15
2	A	1201	PLM	C9-CA-CB-CC
5	A	1207	OLC	C13-C14-C15-C16
5	A	1208	OLC	C7-C8-C9-C10
8	A	1212	OLA	C9-C10-C11-C12
8	A	1212	OLA	O2-C1-C2-C3
8	A	1212	OLA	O1-C1-C2-C3

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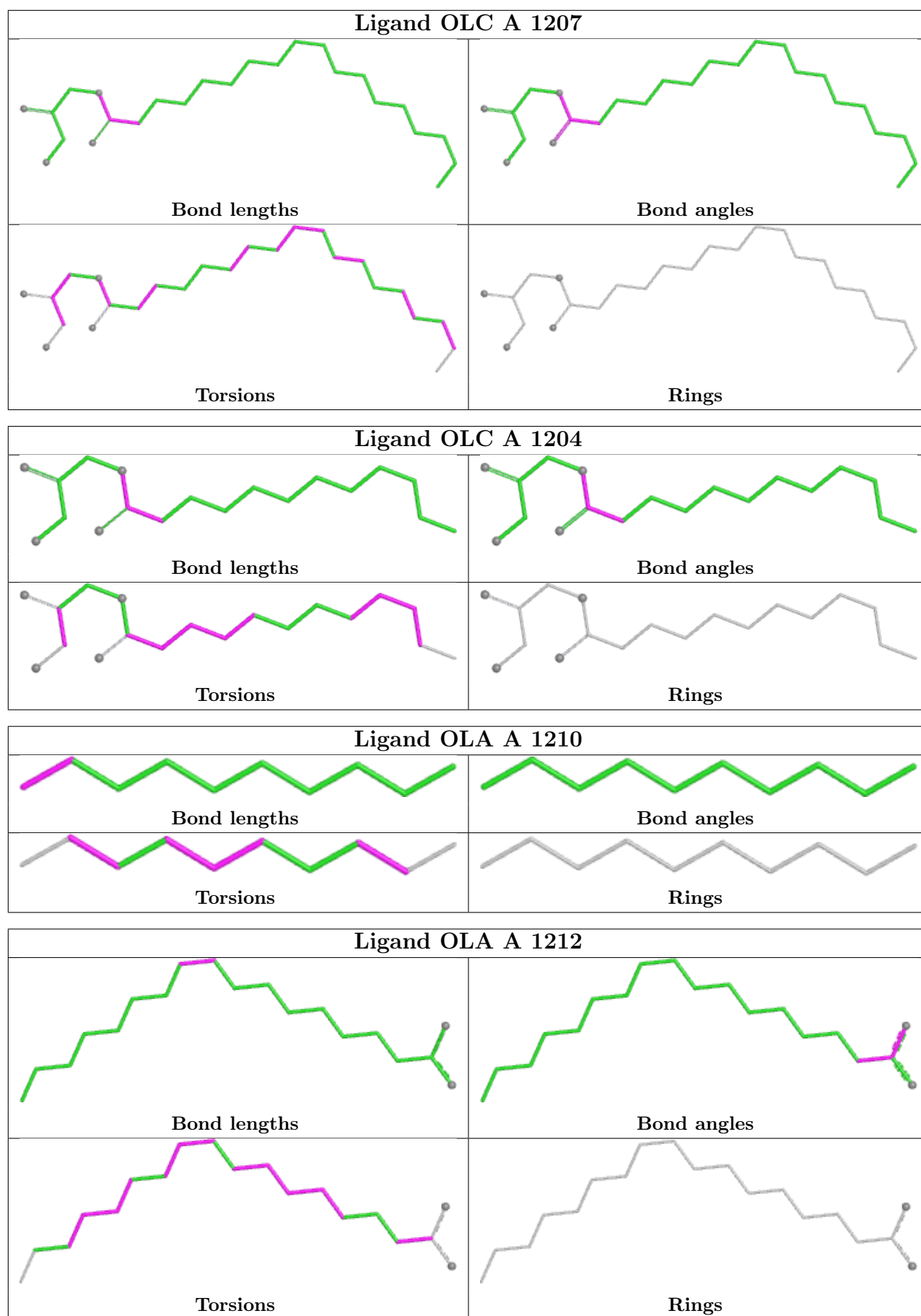
Mol	Chain	Res	Type	Atoms
9	A	1214	DGA	OB1-CB1-OG2-CG2
8	A	1211	OLA	C7-C8-C9-C10
9	A	1214	DGA	OG1-CA1-CA2-CA3
9	A	1213	DGA	OG2-CB1-CB2-CB3
8	A	1211	OLA	C9-C10-C11-C12
5	A	1204	OLC	C2-C3-C4-C5
8	A	1211	OLA	C2-C3-C4-C5
5	A	1204	OLC	O20-C1-C2-C3
2	A	1201	PLM	CA-CB-CC-CD
9	A	1214	DGA	OG2-CB1-CB2-CB3
6	A	1206	PEG	O1-C1-C2-O2
5	A	1204	OLC	C3-C4-C5-C6
4	A	1203	CLR	C21-C20-C22-C23
8	A	1211	OLA	C5-C6-C7-C8
9	A	1214	DGA	OA1-CA1-CA2-CA3
4	A	1203	CLR	C23-C24-C25-C27
9	A	1213	DGA	OA1-CA1-CA2-CA3
5	A	1207	OLC	C7-C8-C9-C10
5	A	1208	OLC	C2-C3-C4-C5

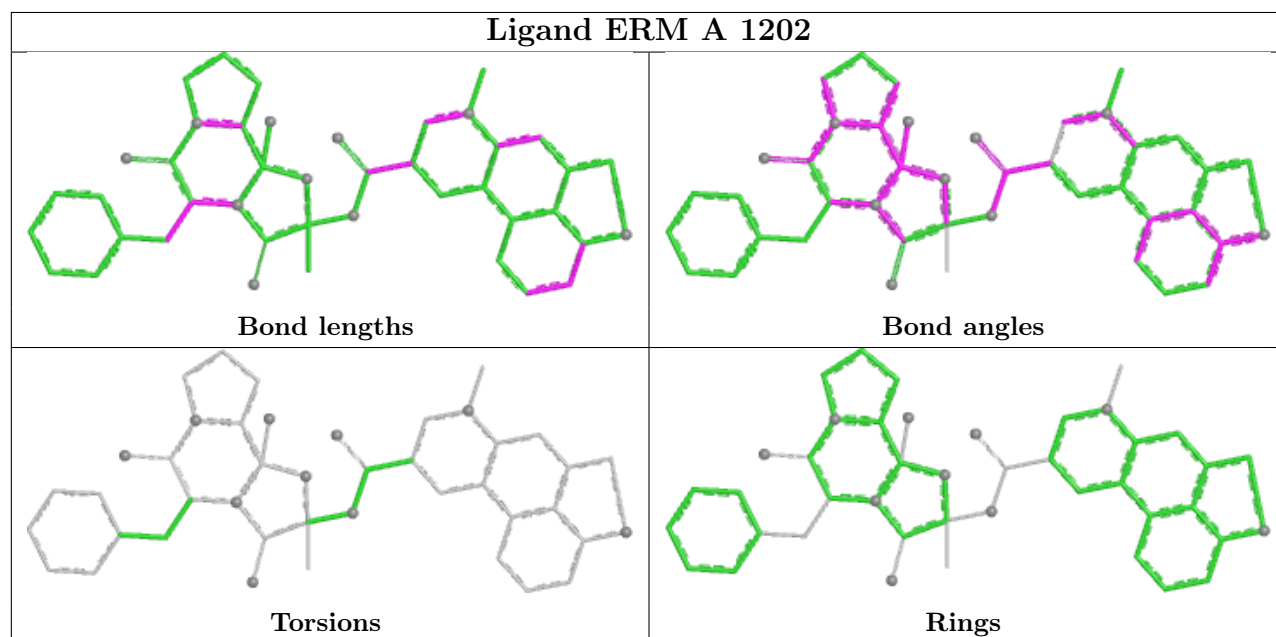
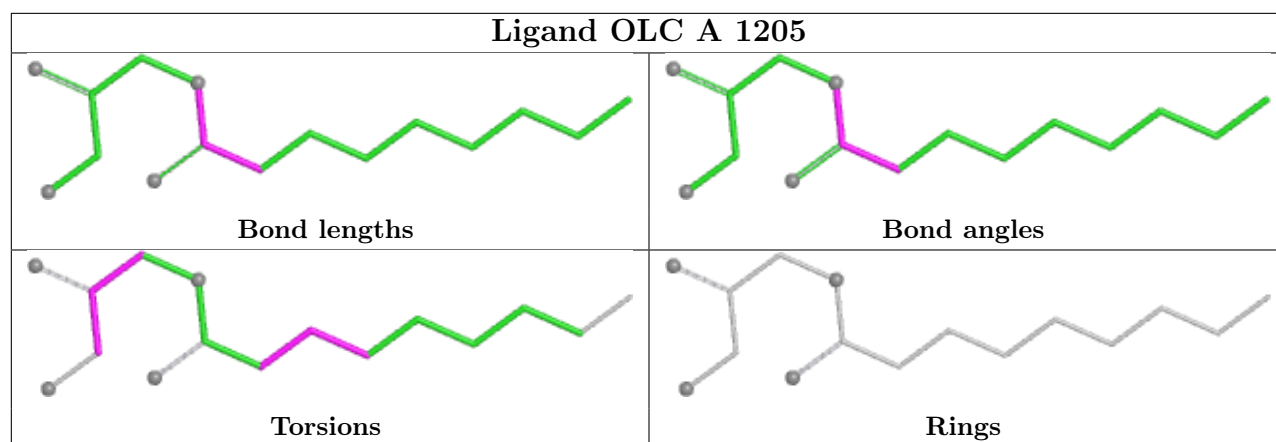
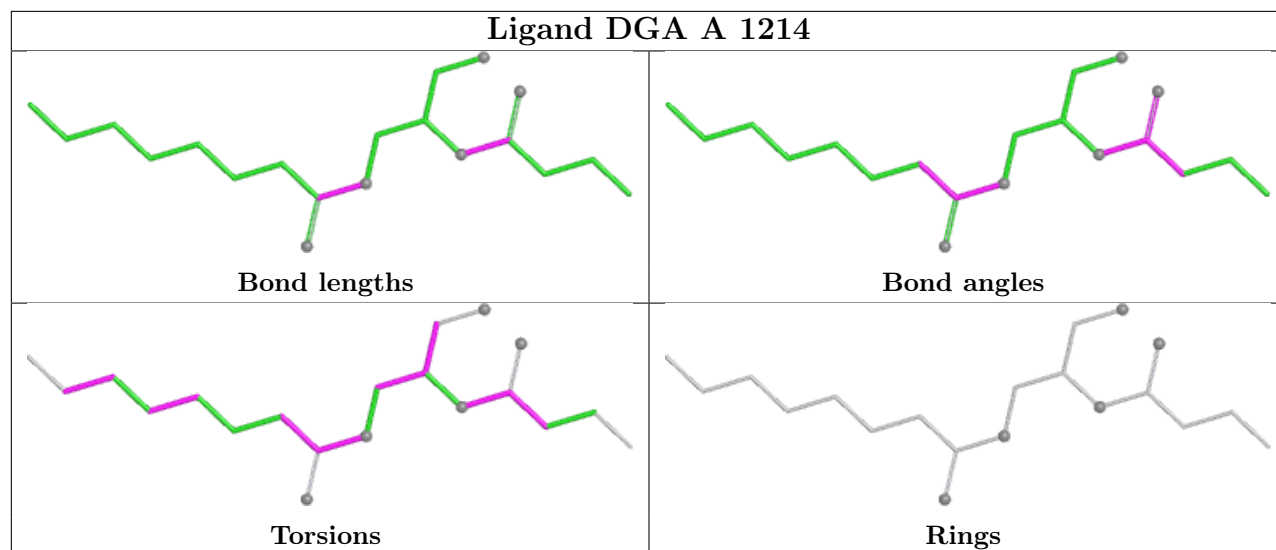
There are no ring outliers.

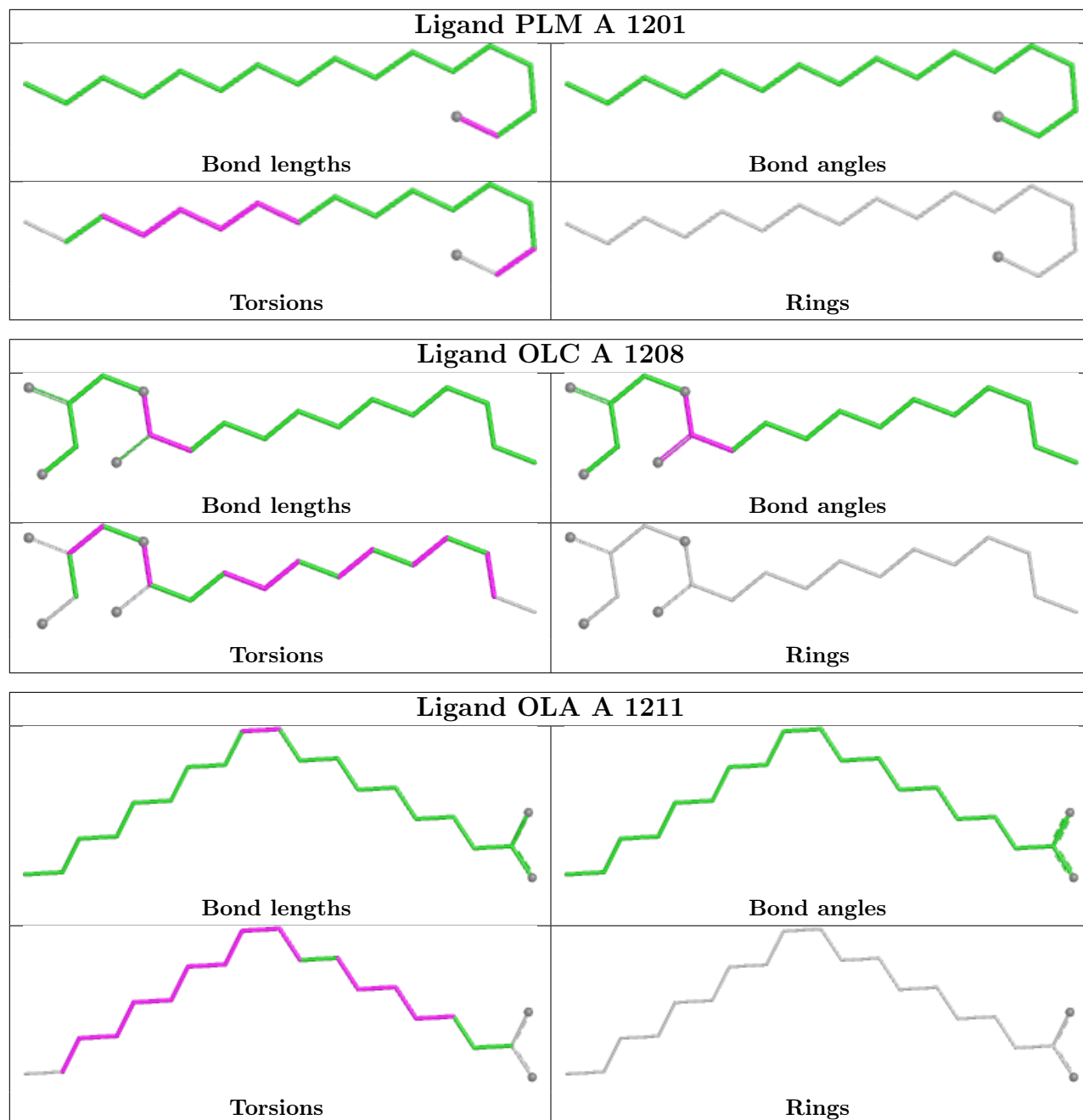
3 monomers are involved in 4 short contacts:

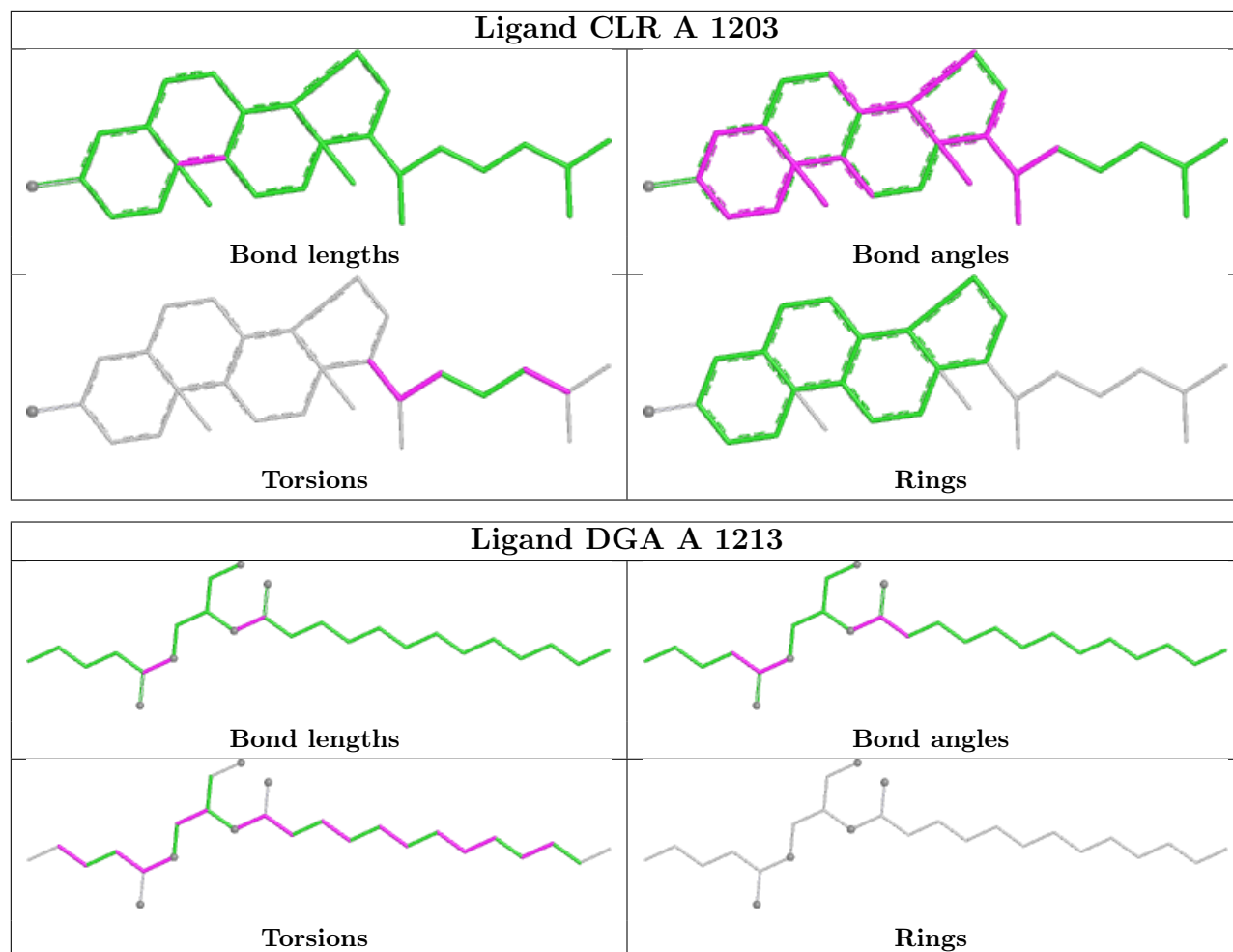
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1207	OLC	2	0
5	A	1204	OLC	1	0
4	A	1203	CLR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	370/430 (86%)	0.79	37 (10%) 12 9	57, 89, 153, 196	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	ALA	4.7
1	A	166	TYR	4.4
1	A	1100	ALA	3.9
1	A	1096	THR	3.9
1	A	120	MET	3.4
1	A	203	ASN	3.1
1	A	381	THR	3.0
1	A	322	ALA	2.9
1	A	1008	GLU	2.9
1	A	1077	LYS	2.9
1	A	119	ALA	2.8
1	A	160	PRO	2.8
1	A	127	LEU	2.7
1	A	164	ASN	2.6
1	A	1065	PHE	2.5
1	A	162	GLN	2.5
1	A	199	VAL	2.5
1	A	1097	THR	2.5
1	A	1061	PHE	2.4
1	A	1032	LYS	2.4
1	A	101	LEU	2.4
1	A	156	ALA	2.4
1	A	1010	LEU	2.4
1	A	117	PHE	2.3
1	A	118	GLU	2.3
1	A	91	TYR	2.3
1	A	1026	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	197	THR	2.3
1	A	1007	TRP	2.2
1	A	1023	ALA	2.2
1	A	205	ILE	2.1
1	A	161	ILE	2.1
1	A	165	GLN	2.1
1	A	1106	LEU	2.1
1	A	316	ILE	2.0
1	A	173	PHE	2.0
1	A	1015	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

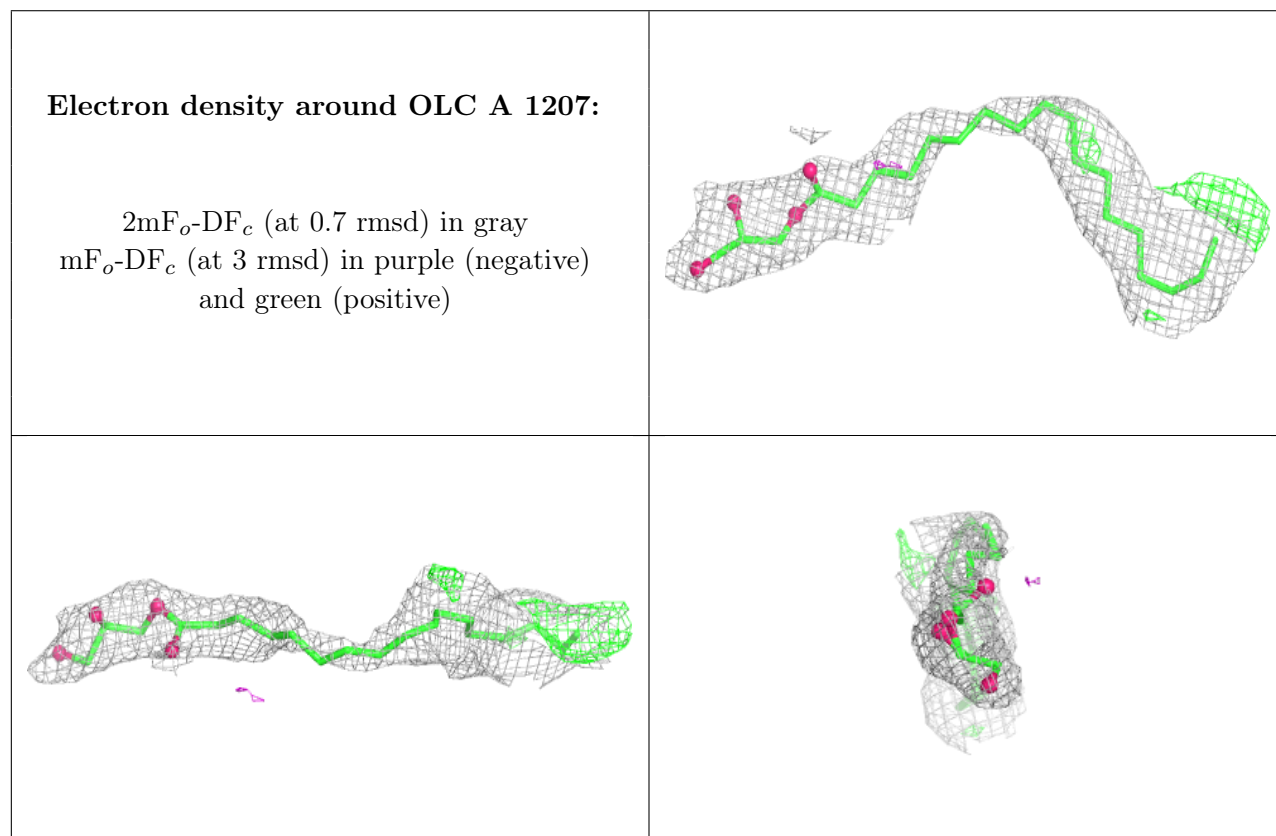
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	TRS	A	1209	8/8	0.52	0.17	133,136,137,138	0
5	OLC	A	1207	25/25	0.75	0.24	99,114,150,154	0
9	DGA	A	1213	26/44	0.78	0.20	108,130,145,147	0
8	OLA	A	1212	19/20	0.82	0.28	101,119,128,128	0
5	OLC	A	1205	16/25	0.84	0.18	70,101,124,125	0
9	DGA	A	1214	20/44	0.84	0.17	104,127,141,146	0
8	OLA	A	1211	20/20	0.85	0.22	77,106,112,113	0
6	PEG	A	1206	7/7	0.87	0.17	94,100,104,107	0
5	OLC	A	1208	19/25	0.90	0.19	80,111,128,130	0
5	OLC	A	1204	19/25	0.93	0.17	58,88,106,108	0
8	OLA	A	1210	10/20	0.93	0.15	84,90,101,101	0
4	CLR	A	1203	28/28	0.94	0.13	72,93,103,105	0
2	PLM	A	1201	17/18	0.94	0.15	100,105,112,113	0

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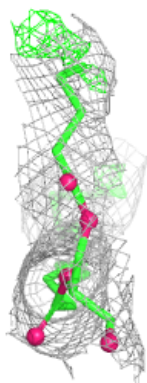
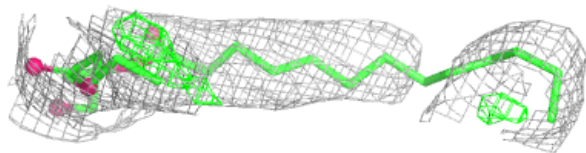
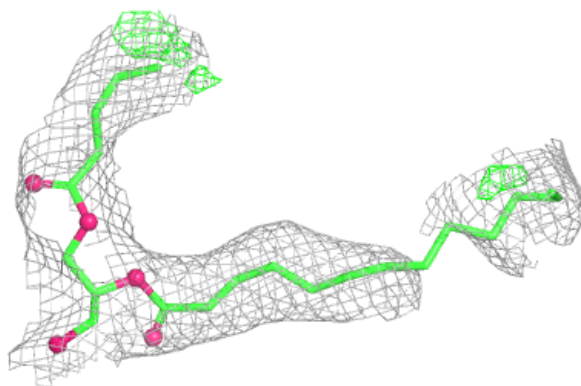
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ERM	A	1202	43/43	0.95	0.10	56,66,79,85	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

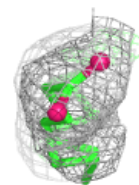
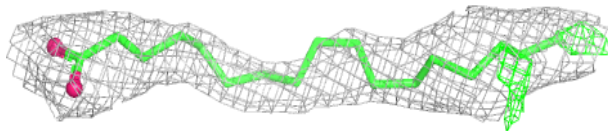
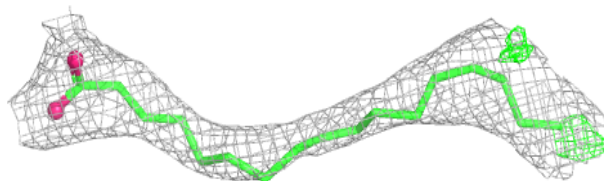


Electron density around DGA A 1213:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

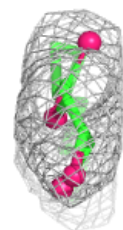
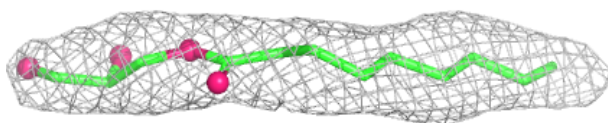
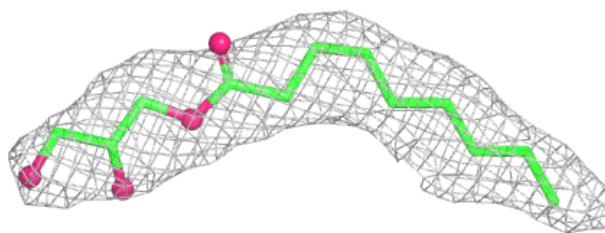
**Electron density around OLA A 1212:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

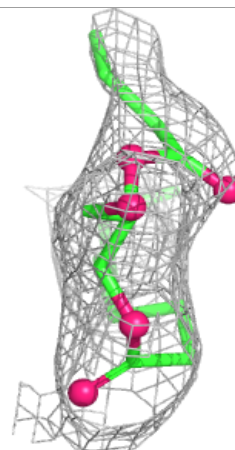
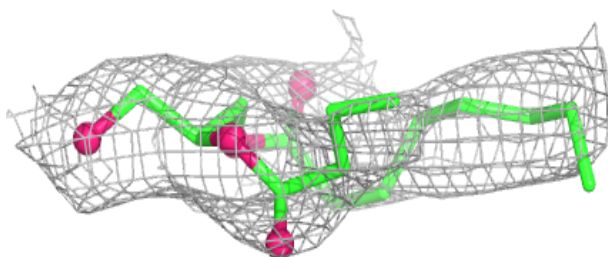
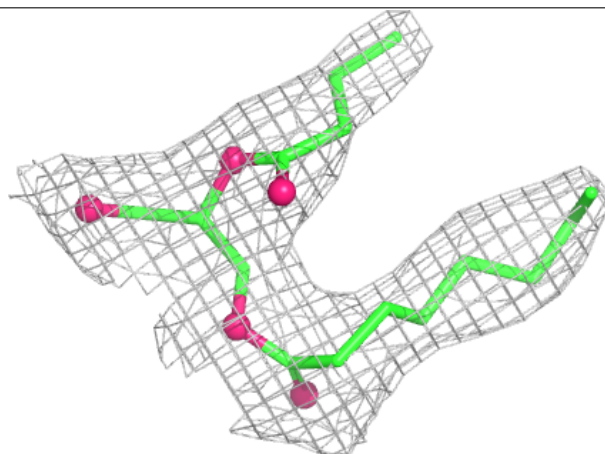


Electron density around OLC A 1205:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

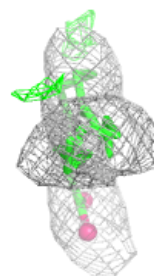
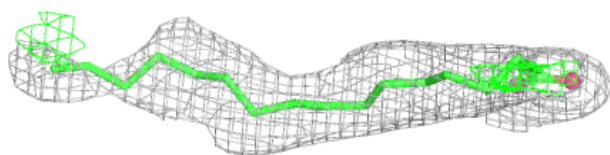
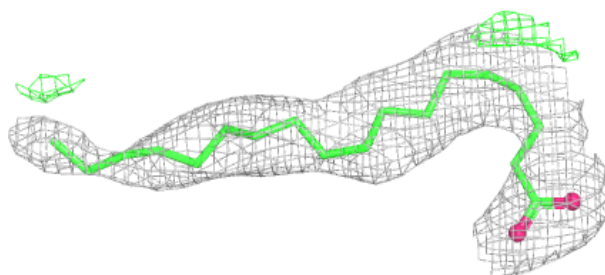
**Electron density around DGA A 1214:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

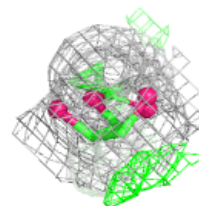
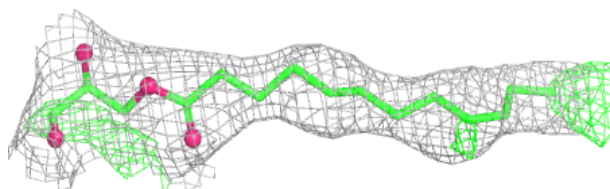
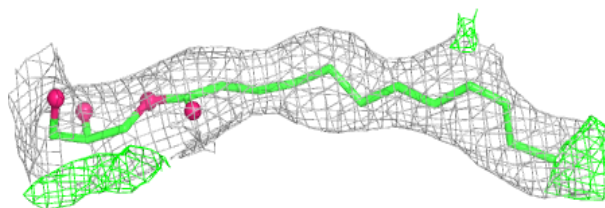


Electron density around OLA A 1211:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

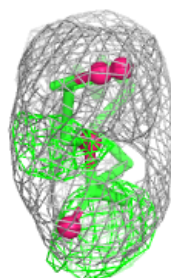
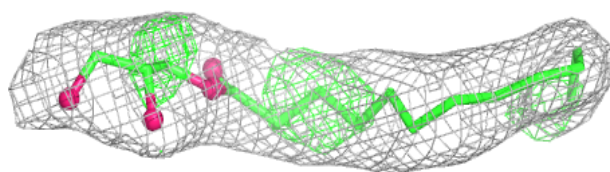
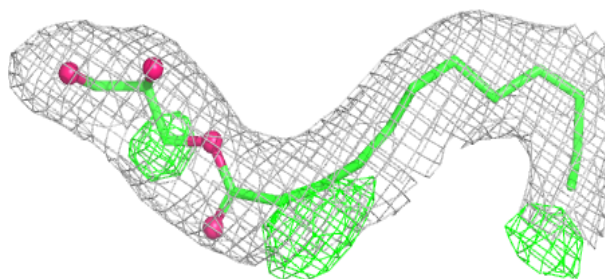
**Electron density around OLC A 1208:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

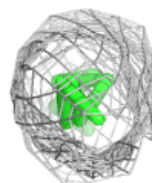
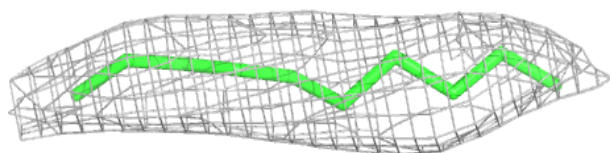
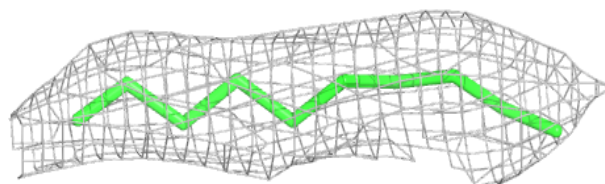


Electron density around OLC A 1204:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

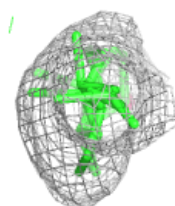
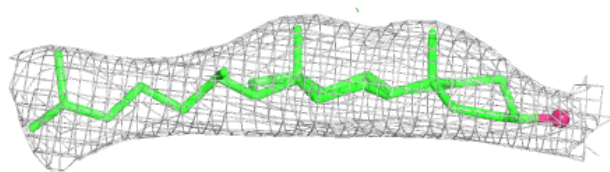
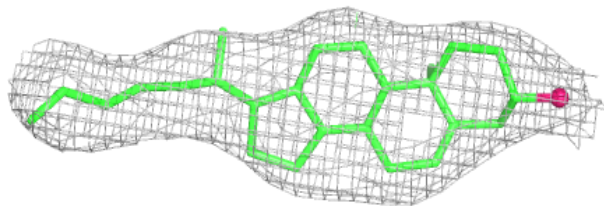
**Electron density around OLA A 1210:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

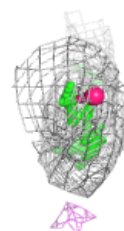
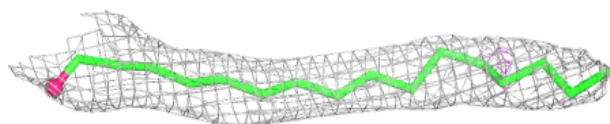
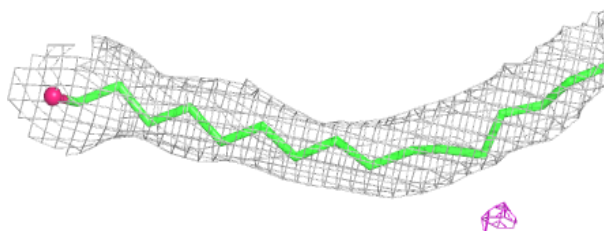


Electron density around CLR A 1203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

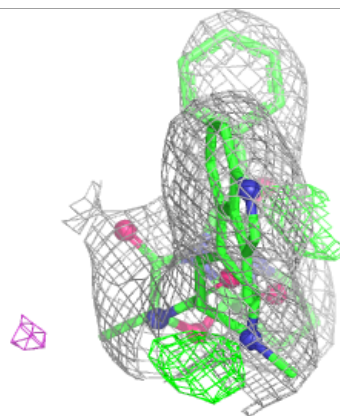
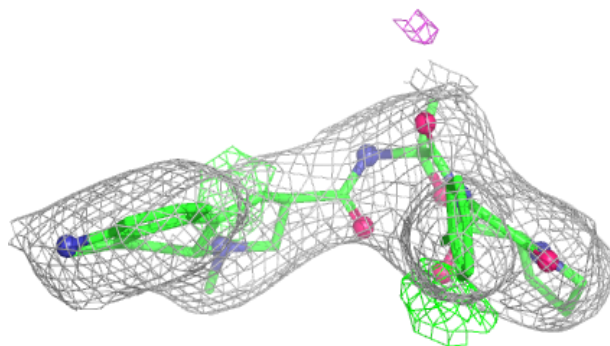
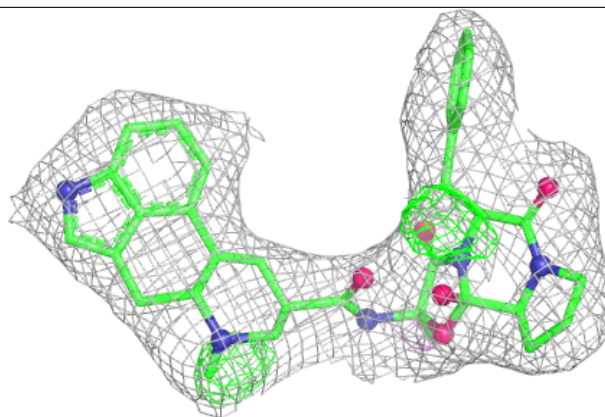
**Electron density around PLM A 1201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ERM A 1202:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.